
X-Ray Data Booklet

Section 1.8 ENERGY LEVELS OF FEW-ELECTRON IONIC SPECIES

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Table 1-4 presents ionization energies for selected few-electron ions with $6 \leq Z \leq 54$. Table 1-5 gives the energies of the resonant $2p$ transitions in hydrogen- and heliumlike ions. The energy values in this section have been generated using the relativistic Hartree-Fock code of I. P. Grant and collaborators [1] with a correction term of the form $A + B/(Z - Q)$ added to bring about agreement with the experimental values known for low atomic numbers. Nuclear size effects, radiative corrections, and the Breit interaction accounting for retardation and the magnetic electron-electron interaction are included in the calculations. The hydrogenic values are uncorrected as they come from the code, but to the accuracy given here, they agree with more detailed calculations. The values in Table 1-4 for Co-, Ni-, and Cu-like ions are based on data from C. E. Moore [2], J. Sugar and A. Musgrove [3], and others referenced therein.

REFERENCES

1. I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, "An Atomic Multiconfigurational Dirac-Fock Package," *Comput. Phys. Commun.* **21**, 207 (1980).
2. C. E. Moore, *Ionization Potentials and Ionization Limits Derived from the Analysis of Optical Spectra*, NBS Pub. NSRDS-NBS 34 (1970).
3. J. Sugar and A. Musgrove, "Energy Levels of Zinc, Zn I through Zn XXX," *J. Phys. Chem. Ref. Data* **24**, 1803 (1995).

X-Ray Data Booklet Table 1-4. Ionization energies, in electron volts, for selected few-electron ionic species.
 Each column is labeled with the number of electrons in the ion before ionization and with the symbol for the neutral atom with the same number of electrons.

| Element | 1 (H) | 2 (He) | 3 (Li) | 4 (Be) | 10 (Ne) | 11 (Na) | 12 (Mg) | 27 (Co) | 28 (Ni) | 29 (Cu) |
|---------|--------|--------|--------|--------|---------|---------|---------|---------|---------|---------|
| 6 C | 490.0 | 392.1 | 64.49 | 47.89 | | | | | | |
| 7 N | 667.1 | 552.1 | 97.89 | 77.48 | | | | | | |
| 8 O | 871.4 | 739.3 | 138.11 | 113.90 | | | | | | |
| 9 F | 1103.1 | 953.9 | 185.18 | 157.15 | | | | | | |
| 10 Ne | 1362.2 | 1195.8 | 239.09 | 207.26 | 21.564 | | | | | |
| 11 Na | 1648.7 | 1465.1 | 299.86 | 264.21 | 47.286 | 5.139 | | | | |
| 12 Mg | 1962.7 | 1761.8 | 367.5 | 328.0 | 80.143 | 15.035 | 7.646 | | | |
| 13 Al | 2304.2 | 2086.0 | 442.0 | 398.7 | 119.99 | 28.447 | 18.828 | | | |
| 14 Si | 2673.2 | 2437.7 | 523.4 | 476.3 | 166.42 | 45.12 | 33.64 | | | |
| 15 P | 3070 | 2816.9 | 611.7 | 560.8 | 220.31 | 65.02 | 51.50 | | | |
| 16 S | 3494 | 3224 | 707.0 | 652.1 | 281.00 | 88.05 | 72.59 | | | |
| 17 Cl | 3946 | 3658 | 809.2 | 750.5 | 348.5 | 114.20 | 96.84 | | | |
| 18 Ar | 4426 | 4121 | 918.4 | 855.8 | 422.8 | 143.46 | 124.24 | | | |
| 19 K | 4934 | 4611 | 1034.6 | 968.0 | 503.9 | 175.82 | 154.75 | | | |
| 20 Ca | 5470 | 5129 | 1157.7 | 1087.3 | 591.9 | 211.28 | 188.38 | | | |
| 21 Sc | 6034 | 5675 | 1288.0 | 1213.6 | 686.6 | 249.84 | 225.13 | | | |
| 22 Ti | 6626 | 6249 | 1425.3 | 1346.9 | 788.2 | 291.50 | 264.98 | | | |
| 23 V | 7246 | 6851 | 1569.7 | 1487.3 | 896.6 | 336.3 | 307.9 | | | |
| 24 Cr | 7895 | 7482 | 1721.2 | 1634.8 | 1011.8 | 384.2 | 354.0 | | | |
| 25 Mn | 8572 | 8141 | 1879.9 | 1789.5 | 1133.8 | 435.2 | 403.2 | | | |
| 26 Fe | 9278 | 8828 | 2045.8 | 1951.3 | 1262.7 | 489.3 | 455.6 | | | |
| 27 Co | 10012 | 9544 | 2218.9 | 2120.4 | 1398.3 | 546.6 | 511.0 | 7.86 | | |
| 28 Ni | 10775 | 10289 | 2399.3 | 2296.7 | 1540.8 | 607.0 | 569.7 | 18.17 | 7.63 | |
| 29 Cu | 11568 | 11063 | 2587.0 | 2480.2 | 1690.2 | 670.6 | 631.4 | 36.83 | 20.29 | 7.73 |
| 30 Zn | 12389 | 11865 | 2782.0 | 2671.1 | 1846.4 | 737.3 | 696.4 | 59.57 | 39.72 | 17.96 |
| 31 Ga | 13239 | 12696 | 2984.4 | 2869.4 | 2009.4 | 807.3 | 764.5 | 86.0 | 63.4 | 30.7 |
| 32 Ge | 14119 | 13557 | 3194 | 3075 | 2179.3 | 880.4 | 835.8 | 115.9 | 90.5 | 45.72 |
| 33 As | 15029 | 14448 | 3412 | 3288 | 2356.0 | 956.8 | 910.3 | 149.2 | 121.2 | 62.3 |
| 34 Se | 15968 | 15367 | 3637 | 3509 | 2539.6 | 1036.3 | 988.1 | 185.5 | 155.4 | 81.7 |
| 35 Br | 16937 | 16317 | 3869 | 3737 | 2730.1 | 1119.1 | 1069.1 | 225.4 | 192.8 | 103.0 |

Table 1-4. Ionization energies, in electron volts, for selected few-electron ionic species. Each column is labeled with the number of electrons in the ion before ionization and with the symbol for the neutral atom with the same number of electrons.

| Element | 1 (H) | 2 (He) | 3 (Li) | 4 (Be) | 10 (Ne) | 11 (Na) | 12 (Mg) | 27 (Co) | 28 (Ni) | 29 (Cu) |
|---------|-------|--------|--------|--------|---------|---------|---------|---------|---------|---------|
| 36 Kr | 17936 | 17296 | 4109 | 3973 | 2927.4 | 1205.2 | 1153.3 | 268.2 | 233.4 | 125.9 |
| 37 Rb | 18965 | 18306 | 4357 | 4216 | 3132 | 1294.5 | 1240.8 | 314.2 | 277.1 | 150.7 |
| 38 Sr | 20025 | 19345 | 4612 | 4467 | 3343 | 1387.2 | 1331.5 | 363.3 | 324.1 | 177.3 |
| 39 Y | 21115 | 20415 | 4876 | 4726 | 3561 | 1483.1 | 1425.6 | 413.6 | 374.0 | 205.9 |
| 40 Zr | 22237 | 21516 | 5147 | 4993 | 3786 | 1582.4 | 1523.0 | 471 | 427.4 | 236.2 |
| 41 Nb | 23389 | 22648 | 5426 | 5268 | 4017 | 1684.9 | 1623.7 | 530 | 483.8 | 268.5 |
| 42 Mo | 24572 | 23810 | 5713 | 5550 | 4256 | 1790.9 | 1727.8 | 592 | 541.7 | 302.6 |
| 43 Tc | 25787 | 25004 | 6008 | 5841 | 4502 | 1900.3 | 1835.2 | 656 | 605.8 | 338.5 |
| 44 Ru | 27033 | 26230 | 6312 | 6140 | 4754 | 2013.0 | 1946.1 | 724 | 671.4 | 376.3 |
| 45 Rh | 28312 | 27487 | 6623 | 6447 | 5014 | 2129.2 | 2060.3 | 795 | 740.1 | 416.0 |
| 46 Pd | 29623 | 28776 | 6943 | 6762 | 5280 | 2248.9 | 2178.0 | 869 | 811.8 | 457.5 |
| 47 Ag | 30966 | 30097 | 7271 | 7086 | 5553 | 2372.0 | 2299.2 | 946 | 886.6 | 500.9 |
| 48 Cd | 32341 | 31451 | 7608 | 7418 | 5834 | 2498.6 | 2423.9 | 1026 | 964.5 | 546.2 |
| 49 In | 33750 | 32837 | 7953 | 7758 | 6121 | 2628.8 | 2552.1 | 1109 | 1045.4 | 593.3 |
| 50 Sn | 35192 | 34257 | 8307 | 8107 | 6415 | 2762.5 | 2683.9 | 1196 | 1129.1 | 642.3 |
| 51 Sb | 36668 | 35710 | 8670 | 8465 | 6717 | 2899.8 | 2819.2 | 1285 | 1215.3 | 693.2 |
| 52 Te | 38177 | 37196 | 9041 | 8832 | 7025 | 3041 | 2958.1 | 1377 | 1306.3 | 746.1 |
| 53 I | 39721 | 38716 | 9421 | 9207 | 7340 | 3185 | 3101 | 1472 | 1399.3 | 800.8 |
| 54 Xe | 41300 | 40271 | 9810 | 9591 | 7663 | 3334 | 3247 | 1571 | 1495.4 | 857.4 |

X-Ray Data Booklet Table 1-5. Transition energies, in electron volts, for transitions from the $n = 2$ states to the $n = 1$ ground state of H- and He- like ions.

| Element | Hydrogenlike | | Heliumlike | |
|---------|--------------|------------|-------------|-------------|
| | $2p_{1/2}$ | $2p_{3/2}$ | $2p\ ^3P_1$ | $2p\ ^1P_1$ |
| 5 B | 255.17 | 255.20 | 202.78 | 205.37 |
| 6 C | 367.5 | 367.5 | 304.3 | 307.8 |
| 7 N | 500.3 | 500.4 | 426.3 | 430.7 |
| 8 O | 653.5 | 653.7 | 568.7 | 574.0 |
| 9 F | 827.3 | 827.6 | 731.5 | 737.8 |
| 10 Ne | 1021.5 | 1022.0 | 914.9 | 922.1 |
| 11 Na | 1236.3 | 1237.0 | 1118.8 | 1126.9 |
| 12 Mg | 1471.7 | 1472.7 | 1343.2 | 1352.3 |
| 13 Al | 1727.7 | 1729.0 | 1588.3 | 1598.4 |
| 14 Si | 2004.3 | 2006.1 | 1853.9 | 1865.1 |
| 15 P | 2301.7 | 2304.0 | 2140.3 | 2152.6 |
| 16 S | 2619.7 | 2622.7 | 2447.3 | 2460.8 |
| 17 Cl | 2958.5 | 2962.4 | 2775.1 | 2789.8 |
| 18 Ar | 3318 | 3323 | 3124 | 3140 |
| 19 K | 3699 | 3705 | 3493 | 3511 |
| 20 Ca | 4100 | 4108 | 3883 | 3903 |
| 21 Sc | 4523 | 4532 | 4295 | 4316 |
| 22 Ti | 4966 | 4977 | 4727 | 4750 |
| 23 V | 5431 | 5444 | 5180 | 5205 |
| 24 Cr | 5917 | 5932 | 5655 | 5682 |
| 25 Mn | 6424 | 6442 | 6151 | 6181 |
| 26 Fe | 6952 | 6973 | 6668 | 6701 |
| 27 Co | 7502 | 7526 | 7206 | 7242 |
| 28 Ni | 8073 | 8102 | 7766 | 7806 |
| 29 Cu | 8666 | 8699 | 8347 | 8392 |
| 30 Zn | 9281 | 9318 | 8950 | 8999 |
| 31 Ga | 9917 | 9960 | 9575 | 9628 |
| 32 Ge | 10575 | 10624 | 10221 | 10280 |
| 33 As | 11255 | 11311 | 10889 | 10955 |
| 34 Se | 11958 | 12021 | 11579 | 11652 |
| 35 Br | 12682 | 12753 | 12292 | 12372 |
| 36 Kr | 13429 | 13509 | 13026 | 13114 |
| 37 Rb | 14199 | 14288 | 13783 | 13880 |
| 38 Sr | 14990 | 15090 | 14562 | 14669 |
| 39 Y | 15805 | 15916 | 15364 | 15482 |
| 40 Zr | 16643 | 16765 | 16189 | 16318 |
| 41 Nb | 17503 | 17639 | 17036 | 17178 |
| 42 Mo | 18387 | 18537 | 17907 | 18062 |
| 43 Tc | 19294 | 19459 | 18800 | 18971 |
| 44 Ru | 20224 | 20406 | 19717 | 19904 |
| 45 Rh | 21178 | 21377 | 20658 | 20861 |
| 46 Pd | 22156 | 22374 | 21622 | 21843 |
| 47 Ag | 23157 | 23396 | 22609 | 22851 |
| 48 Cd | 24183 | 24444 | 23621 | 23884 |
| 49 In | 25233 | 25518 | 24657 | 24942 |
| 50 Sn | 26308 | 26617 | 25717 | 26027 |